Long-time integration of non-stiff and oscillatory Hamiltonian systems

Ernst Hairer

Section de Mathématiques, Université de Genève, CH-1211 Genève 4, Switzerland

Abstract. For the long-time integration of Hamiltonian systems (e.g., planetary motion, molecular dynamics simulation) much insight can be gained with "backward error analysis". For example, it explains why symplectic integrators nearly conserve the energy, and why they have at most a linear error growth for integrable systems. This theory breaks down in the presence of high oscillations, when the product of the step size with the highest frequency is not small. In the situation, where the high oscillations originate from a linear part in the differential equation, the theory of "modulated Fourier expansion" yields much information on the long-time behavior of analytic and numerical solutions, in particular for large step sizes.

After a short review on backward error analysis, the main ideas and results of modulated Fourier expansions are presented. They are then applied to get new insight into the distribution of the modal energy spectrum of the Fermi–Pasta–Ulam problem.

Keywords: Hamiltonian systems, symplectic methods, exponential integrators, long-time integration, geometric numerical integration, backward error analysis, modulated Fourier expansion, Fermi–Pasta–Ulam problem.
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INTEGRATION OF HAMILTONIAN SYSTEMS

Although many of the presented statements remain valid for general Hamiltonian systems, we restrict ourselves to problems of the form

$$\ddot{q} = f(q), \qquad f(q) = -\nabla U(q), \tag{1}$$

where $U(q)$ is a sufficiently smooth potential. Introducing the momentum $p = \dot{q}$ as new variable, we get a first order Hamiltonian system. It is a classical result by Poincaré that its flow is symplectic. Moreover, it can be checked by differentiation that the Hamiltonian

$$H(p,q) = \tfrac{1}{2}\, p^T p + U(q) \tag{2}$$

is preserved along solutions of the system.

The most natural discretization of such a system is

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n), \qquad p_n = \frac{q_{n+1} - q_{n-1}}{2h}, \tag{3}$$

which is referred to as the Störmer–Verlet method (leap-frog in the context of partial differential equations). Written as a one-step method $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$, it is of order two, symplectic, symmetric, and time-reversible (see [1, 2]).

BACKWARD ERROR ANALYSIS

The idea of backward error analysis is to find smooth functions $\widetilde{p}(t), \widetilde{q}(t)$ that

- interpolate the numerical solution (p_n, q_n) (obtained with fixed step size h), and
- are solution of a modified differential equation with a vector field written as a formal series in powers of h.

The construction of the modified differential equation is straight-forward for general differential equations and for general one-step methods. The success of backward error analysis lies in the fact that the modified differential equation inherits geometric properties of the problem and the method. E.g., for the system (1) and the method (3) we have the following result.

Theorem. *There exist functions $H_j(p,q)$ such that the solution $\widetilde{p}(t), \widetilde{q}(t)$ of the Hamiltonian system*

$$\begin{aligned} \dot p &= -\nabla_q \widetilde H(p,q) \\ \dot q &= \nabla_p \widetilde H(p,q) \end{aligned} \qquad \textit{with} \qquad \widetilde H(p,q) = \tfrac{1}{2} p^T p + U(q) + h^2 H_2(p,q) + \ldots + h^{2N} H_{2N}(p,q) \tag{4}$$

and initial values p_n, q_n at $t_n = nh$ satisfies

$$\|p_{n+1} - \widetilde p(t_n + h)\| + \|q_{n+1} - \widetilde q(t_n + h)\| \le C_N h^{2N+2}.$$

The near conservation of energy is a simple consequence of this result: along the solution of the modified differential equation (4), the modified Hamiltonian is a conserved quantity so that also $\widetilde H\big(p_{n+1}, q_{n+1}\big) = \widetilde H\big(p_n, q_n\big) + \mathcal{O}(h^{2N+2})$. Summing up yields $\widetilde H\big(p_n, q_n\big) = \widetilde H\big(p_0, q_0\big) + \mathcal{O}(t_n h^{2N+1})$ and

$$H\big(p_n, q_n\big) = H\big(p_0, q_0\big) + \mathcal{O}(h^2) + \mathcal{O}(t_n h^{2N+1})$$

as long as the numerical solution stays in a compact set. This means that the energy is conserved up to an error of size $\mathcal{O}(h^2)$ on time intervals of length $t_n \le C_N h^{-2N+1}$. For exponentially small error estimates and for further applications of backward error analysis we refer to the monographs [1, 3].

In the presence of *high oscillations*, e.g., for the harmonic oscillator $H(p,q) = \frac{1}{2} p^2 + \frac{1}{2} \omega^2 q^2$, the exact and numerical solutions depend on ωh rather than only on h. Therefore, the above derivation gives in fact

$$H\big(p_n, q_n\big) = H\big(p_0, q_0\big) + \mathcal{O}((\omega h)^2) + \mathcal{O}(t_n \omega (\omega h)^{2N+1})$$

where ω is the highest frequency in the system. Hence, backward error analysis does not give any information on the long-time behaviour for step sizes such that $\omega h \approx 1$.

MODULATED FOURIER EXPANSION

Here we focus on problems with highly oscillatory solutions. A typical example is the motion of a chain, where stiff harmonic springs (with frequency $\omega \gg 1$) alternate with soft nonlinear springs. The differential equation becomes

$$\begin{aligned} \ddot y_0 &= -\nabla_{y_0} U(y_0, y_1) \\ \ddot y_1 + \omega^2 y_1 &= -\nabla_{y_1} U(y_0, y_1) \end{aligned} \qquad \text{or} \qquad \ddot y + \Omega^2 y = -\nabla U(y)$$

where $y_0 \in \mathbb{R}^m$ are the displacements from the position of rest of the stiff springs, and $y_1 \in \mathbb{R}^m$ represent their expansion/compression. An important feature of such systems is that not only the total energy $H(y, \dot y)$ is conserved, but also the oscillatory energy ($\dot y_{1,j}$ denotes the jth component of y_1)

$$I(y_1, \dot y_1) = I_1 + I_2 + \ldots + I_m = const + \mathcal{O}(\omega^{-1}), \qquad I_j = \tfrac{1}{2}(\dot y_{1,j}^2 + \omega^2 y_{1,j}^2)$$

is nearly conserved up to oscillations of size $\mathcal{O}(\omega^{-1})$ over exponentially long (in ω) time intervals (see [4]). This is illustrated in Figure 1 for the case $m = 3$ and $\omega = 30$: the left picture presents the exact solution, and the right picture is the Störmer–Verlet solution with large step size satisfying $h\omega = 0.5$ over a much longer time interval.

The technique of modulated Fourier expansion permits us to explain the long-time behavior of analytic as well as numerical solutions for such types of highly oscillatory differential equations. The presence of two time scales (fast time ωt in oscillations of the stiff harmonic springs and slow time t due to the soft nonlinear coupling) motivates for the analytic solution the ansatz

$$y(t) = \sum_{k \in \mathbb{Z}} z^k(t)\, \mathrm{e}^{\mathrm{i} k \omega t} = \sum_{k \in \mathbb{Z}} \begin{pmatrix} z_0^k(t) \\ z_1^k(t) \end{pmatrix} \mathrm{e}^{\mathrm{i} k \omega t}, \tag{5}$$

where the coefficient functions $z_j^k(t)$ are smooth with derivatives bounded uniformly in $\omega \ge 1$. For the numerical solution we search for a function $\widetilde y(t)$ as in (5) but with coefficient functions $\widetilde z_j^k(t)$, such that in the spirit of backward error analysis, the numerical solution formally satisfies $y_n = \widetilde y(t_n)$. This is possible for so-called exponential integrators

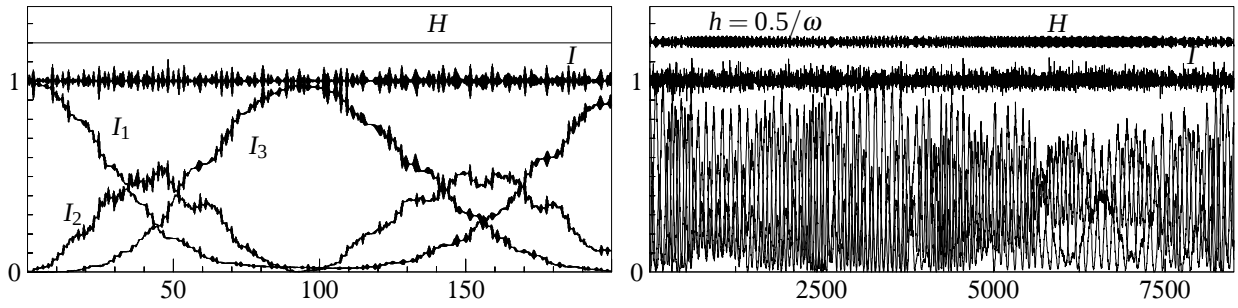

FIGURE 1. Exact solution (left) and numerical solution (right)

which discretize the linear part of the differential equation without error, and also for the Störmer–Verlet method, when it is interpreted as an exponential integrator applied to a system with modified frequencies. Let us sketch the different steps for a proof of near conservation of the total and oscillatory energies by the numerical integrator:

- prove the existence of smooth functions $z_j^k(t)$ (resp. $\widetilde{z}_j^k(t)$) on intervals of length ω,
- find a Hamiltonian system for $z^k(t)$ of the exact solution,
- find a *modified Hamiltonian* system for $\widetilde{z}^k(t)$ of the numerical solution,
- study formal invariants for both systems,
- reinterpret the results in terms of y_n.

In this way, it is possible to prove for an exponential integrator (and for the Störmer–Verlet method) that under suitable numerical non-resonance conditions the total and oscillatory energies are nearly conserved over long time intervals. Details of the proof are given in [5, 1]. An extension of the results to finitely many high frequencies (with possible resonances) is elaborated in [6], and for the discretized nonlinearly perturbed wave equation in [7, 8].

Recently, modulated Fourier expansions have been used for analyzing heterogeneous multiscale methods [9], and for solving differential-algebraic equation arising in circuit theory (talk at SciCADE09 by Arieh Iserles).

APPLICATION TO THE FERMI–PASTA–ULAM PROBLEM

We consider a long chain of particles interacting through identical nonlinear springs:

$$\ddot{q}_n - (q_{n+1} - 2q_n + q_{n-1}) = V'(q_{n+1} - q_n) - V'(q_n - q_{n-1})$$

with potential $V(u) = u^3/3$ and periodic boundary conditions $q_{2N} = q_0$. With the discrete Fourier coefficients

$$y = \big(y_j\big)_{j=-N}^{N-1}, \qquad q_n = \sum_{j=-N}^{N-1} y_j \, \mathrm{e}^{\mathrm{i}jn\pi/N},$$

we obtain the Hamiltonian system

$$\ddot{y}_j + \omega_j^2 y_j \;= -\,\mathrm{i}\,\omega_j \sum_{j_1+j_2=j \bmod 2N} (-1)^{(j_1+j_2-j)/(2N)}\, \omega_{j_1}\, \omega_{j_2}\, y_{j_1} y_{j_2}$$

with frequencies $\omega_j = 2\sin(\frac{j\pi}{2N})$ for $j = -N, \ldots, N-1$. This problem is extensively studied over many years and a recent Lecture Notes in Physics [10] gives a "status report" on the main developments. One of the interesting questions is the study of the long-time behavior of the harmonic energies

$$E_j(t) = \tfrac{1}{2}\big(|\dot{y}_j(t)|^2 + \omega_j^2\,|y_j(t)|^2\big)$$

when only one (or a few) low frequency modes are excited in the initial state: $E_1(0) = \varepsilon^2$ and $E_j(0) = 0$ for $j = 2, \ldots, N$. The frequencies ω_j are dense in the interval $[-2, 2]$, and it is a priori not evident, if the approach by modulated Fourier

expansions, which is based on the separation of *two* time scales, will be useful. Numerical experiments (see Figure 2) and the fact that $\omega_k + \omega_\ell - \omega_{k+\ell} = \mathcal{O}(N^{-3})$ for small k and ℓ, suggest the existence of an expansion of the form

$$y_j(t) = \sum_{k=-N}^{N-1} z_j^k(\tau)\, \mathrm{e}^{\mathrm{i}\omega_k t} \qquad \text{with} \quad \tau = N^{-3}t.$$

The main difference to the expansion in the previous section is that the dominant frequencies ω_k are in resonance, so that products of $\mathrm{e}^{\mathrm{i}\omega_k t}$ need not be considered in the expansion. A formal analysis shows that for ε significantly smaller than N^{-2}, the harmonic energies for the analytic solution satisfy

$$E_j(t) = \varepsilon^{2j} N^{4j-4} |u_j(\tau)|^2 + \mathcal{O}(\varepsilon^{2j} N^{4j-6}) + \mathcal{O}(\varepsilon^{2j+2} N^{4j}) \tag{6}$$

where (with the abbreviation $\alpha(k,\ell) = \omega_k + \omega_\ell - \omega_{k+\ell}$)

$$u_1(\tau) = 1, \qquad u_2(\tau) = \frac{4}{\pi^2}\Big(\mathrm{e}^{\mathrm{i}\alpha(1,1)\tau} - 1\Big), \qquad u_3(\tau) = \frac{12}{\pi^4}\Big(\mathrm{e}^{\mathrm{i}(\alpha(1,1)+\alpha(1,2))\tau} - 1\Big) - \frac{16}{\pi^4}\Big(\mathrm{e}^{\mathrm{i}\alpha(1,2)\tau} - 1\Big).$$

For the numerical solution obtained by the Störmer–Verlet method (with $h < 1$) we have (6) with, e.g.,

$$u_2(\tau) = \frac{4}{\pi^2(1-h^2)}\Big(\mathrm{e}^{\mathrm{i}\widetilde{\alpha}\tau} - 1\Big), \qquad \widetilde{\alpha} = \alpha(1,1)(1-h^2) + \mathcal{O}(N^{-2}).$$

These formulas agree extremely well with numerical experiments (see Figure 2, where the step size is such that $h\,\omega_{\max} = 1.6$). In fact, plots of the leading term in (6) cannot be distinguished from the exact energies (for analytic as well as numerical solution). These results are taken from a joint-work with Christian Lubich, which is in preparation.

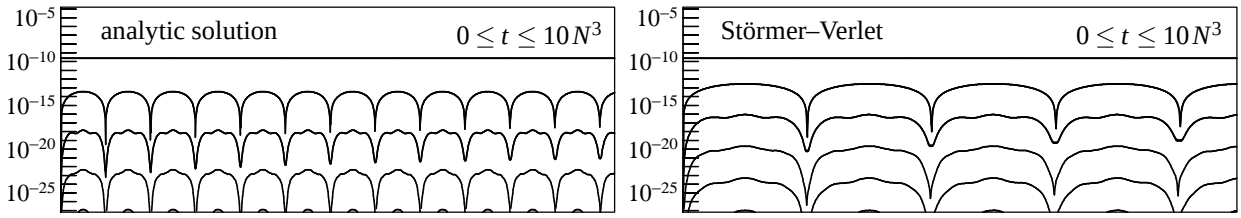

FIGURE 2. Harmonic energies $E_j(t)$ for $j = 1, 2, \ldots$ as function of time, $N = 32$, $\varepsilon = N^{-3}$.

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